

SECURITY

AD-A250 642



DOCUMENTATION PAGE

1a. REPO UNCLASSIFIED		1b. RESTRICTIVE MARKINGS													
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited.													
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE		5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR- 92 0271													
4. PERFORMING ORGANIZATION REPORT NUMBER(S) DTIC ELECTE		6. NAME OF MONITORING ORGANIZATION Air Force Office of Scientific Research													
6a. NAME OF PERFORMING ORGANIZATION University of Wisconsin		7b. ADDRESS (City, State and ZIP Code) Directorate of Mathematical & Information Sciences, Bolling AFB DC 20332-6448													
6c. ADDRESS (City, State and ZIP Code) 750 University Avenue Madison, WI 53706		7d. ADDRESS (City, State and ZIP Code) Directorate of Mathematical & Information Sciences, Bolling AFB DC 20332-6448													
8a. NAME OF FUNDING/SPONSORING ORGANIZATION AFOSR	8b. OFFICE SYMBOL (If applicable) NM	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER AFOSR-89-0220													
8c. ADDRESS (City, State and ZIP Code) Bolling AFB DC 20332-6448		10. SOURCE OF FUNDING NOS. <table border="1"><tr><td>PROGRAM ELEMENT NO. 61102F</td><td>PROJECT NO. 2304</td><td>TASK NO. A3</td><td>WORK UNIT NO.</td></tr></table>		PROGRAM ELEMENT NO. 61102F	PROJECT NO. 2304	TASK NO. A3	WORK UNIT NO.								
PROGRAM ELEMENT NO. 61102F	PROJECT NO. 2304	TASK NO. A3	WORK UNIT NO.												
11. TITLE (Include Security Classification) New Transient and Pseudo-Transient Algorithms for Viscoelastic Materials (u)															
12. PERSONAL AUTHOR(S) David S. Malkus															
13a. TYPE OF REPORT Final Technical	13b. TIME COVERED FROM 12/15/88-6/14/91	14. DATE OF REPORT (Yr., Mo., Day) 92-3-4	15. PAGE COUNT 6												
16. SUPPLEMENTARY NOTATION															
17. COSATI CODES <table border="1"><tr><th>FIELD</th><th>GROUP</th><th>SUB. GR.</th></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr></table>		FIELD	GROUP	SUB. GR.										18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
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19. ABSTRACT (Continue on reverse if necessary and identify by block number) <p>The principal investigator, D. S. Malkus, his post-doctoral associate, and Ph.D. students worked on three projects related to AFOSR research: (1) Planar viscoelastic flows of fluids with integral constitutive equations. The purpose of the project was to develop new algorithms for flows of non-Newtonian fluids and use them to study polymer-processing flows. (2) Simulation and analysis of differential infrared thermographic stress analysis -- SPATE. A consistent thermodynamic theory of viscoplasticity was developed and methods for the experimental determination of model parameters were proposed. The consequence of viscoplastic behavior on differential thermography was studied, by simulating the SPATE stress analysis system. (3) Optimal mass in the finite element method. The purpose of the project was to explore the feasibility and usefulness of quadrature-based optimal mass matrix lumping techniques for higher-order finite element schemes, where they often produce indefinite but diagonal mass matrices.</p>															
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS <input type="checkbox"/>		21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED													
22a. NAME OF RESPONSIBLE INDIVIDUAL Dr. Marc Jacobs		22b. TELEPHONE NUMBER (Include Area Code) (202) 767-4939	22c. OFFICE SYMBOL NM												

NEW TRANSIENT AND PSEUDO-TRANSIENT ALGORITHMS FOR DISCOELASTIC MATERIALS¹

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4 March 1992

Final Technical Report for Grant AFOSR 89-0220 Covering Period

15 DEC 88 - 14 JUN 91

DISTRIBUTION: unclassified/unlimited

Prepared for

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
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Bolling AFB DC 20332-6448

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Research Progress

The principal investigator, D. S. Malkus, his post-doctoral associate, and Ph.D. students worked on three projects related to AFOSR research. What follows is a description of progress made during the reporting period:

Planar Viscoelastic Flows of Fluids with Integral Constitutive Equations: The purpose of the project was to develop new algorithms for flows of non-Newtonian fluids and use them to study polymer-processing flows. In recent work, Malkus and co-workers have shown that process-disrupting instabilities in shear flows can be modelled by constitutive equations with non-monotone shear stress. A number of interesting phenomena that appear to be related to or interpretable as "slip" or "apparent slip" can be reproduced by such models without invoking any mechanism for the loss of adhesion at the walls. Rather, the polymer system changes state in a thin layer near the wall, giving the appearance of a slip layer. Molecular mechanisms for the change of state are not clearly understood, though a number of constitutive equations derived from molecular arguments exhibit the required non-monotonicity; this feature was long believed to represent a defect of the model. Malkus' recent research is aimed at convincing rheologists to reconsider this assessment, and this is a subject of great controversy in the rheological community. We can currently make some fairly convincing arguments based on dynamical systems (finite and infinite dimensional) to elucidate this "material property hypothesis" of slip-like phenomena. The dynamical systems can be approximated and simulated on a Macintosh II, using a fairly straight-forward Pascal code that takes advantage of the powerful interactive and graphical capabilities.

In other computations, we have been investigating the effects of geometric complexity, such as reentrant corners, using the existing steady, planar flow algorithm, developed during prior AFOSR-sponsored research (A FAST ALGORITHM FOR NON-NEWTONIAN FLOW—AFOSR Grant 85-0141). There is a great deal of interest in understanding the role of corner singularities in non-Newtonian flows; we have been studying flows through contractions and over transverse slots using highly refined meshes with many thousands of finite elements. We have been investigating the effects on the flow field of rounding corners symmetrically and asymmetrically. Our computations are always accompanied by posterior error analyses to verify convergence rates and assess the effect of various singularities on convergence rate with mesh refinement. Such studies are also very relevant to the study of slip-like phenomena. For appropriately determined flow fields, it is possible to have a situation in which

one-dimensional analysis would predict the development of a slip layer in a small neighborhood of the corner. Our hope is that the steady flow algorithm can be modified in the neighborhood of the layer to produce steady, layered solutions and observe the effect of such a layer on the large-scale flow field (we have reason to anticipate that the effect may be large).

An important thrust of our current research was to develop algorithms for planar and axisymmetrical geometries that generalize successful one-dimensional algorithms. One of the lessons of the one-dimensional analysis is that the full dynamics of the system -- as opposed to *a priori* assumption of stationarity -- must be simulated in order to obtain a well-posed problem when the shear stress is non-monotone. Development of transient algorithms will also allow us to investigate the stability of spurt solutions to higher dimensional disturbances. The numerical approach we are developing was described in the original proposal. We have developed the proposed technique of a Lagrangian difference scheme along streamlines that use an "Oldroyd Difference Quotient." The "ODQ" algorithm has been tested in an axisymmetric problem, the drawing of a viscoelastic filament. Though much of the complexity of the higher-dimensional flows is inherent in this problem, it can be solved in one space dimension with an added continuity equation governing the free surface of the filament. The complete realization of the research proposed in the original proposal will be to use the "ODQ" transient integrator to develop nearly steady slip solutions with a closely matched differential constitutive equation and the switch to the associated integral model for the final iterations to a converged steady state, as described in the proposal. This research was in progress when the current grant expired.

Simulation and Analysis of Differential Infrared Thermographic Stress Analysis -- SPATE: In recent work, Malkus and R. Cornwell (AFOSR R.A.) developed a consistent thermodynamic theory of viscoplasticity and proposed methods for the experimental determination of model parameters; of particular interest is the relaxation spectrum of the heat capacity term in the energy equation. We investigated the consequence of viscoplastic behavior on differential thermography, by simulating the SPATE stress analysis system. The theory behind differential thermography only rigorously applies to linearly elastic material, but material failure mechanisms often involve plastic deformation, stress relaxation, and creep. How such mechanisms would be sensed by differential thermography, how the device could be calibrated, and what the accuracy of such measurements would be were addressed. Our major conclusion was that differential thermography could be used to measure stresses by thermal emission for inelastic materials, if care is taken to separate the effects of thermal dissipation drift. The code was tested, vectorized and optimized for a Cray YMP

and was being used to perform full simulation of geometrically realistic test specimens at the time the current grant expired.

Optimal Mass in the Finite Element Method: The purpose of the project is to explore the feasibility and usefulness of quadrature-based optimal mass matrix lumping techniques for higher-order finite element schemes, where they often produce indefinite but diagonal mass matrices. The method seems to offer significant computational savings in both direct integration of the equations of motion and modal synthesis, but it poses intriguing mathematical challenges, in that many algorithms structural analysts employ assume the positive definiteness of the mass matrix. With some fancy footwork, many direct integration and eigensolution methods can be made to work with indefinite mass; it is not yet clear how indefinite mass would interact with such useful engineering expedients as condensation, substructuring, and component mode synthesis. The major thrust of this project is to find out whether this fancy footwork is worth the effort in practical engineering analysis. During the reporting period Malkus, Y.-C. Tsai, and T.-P. Tsai (Engineering Mechanics Department Teaching Assistant) have demonstrated that popular ad-hoc lumping schemes devised to preserve positive definiteness are suboptimal in terms of convergence rate in the standard norms. It appears that in modal analysis quadrature-based lumping schemes and their attendant indefiniteness are necessary to retain accuracy.

Our current research has focussed on the translation of the knowledge gained from investigation of the discrete spectrum to the development of time-integration schemes that take advantage of the diagonalization of the mass matrix by optimal lumping. Such schemes exist were developed by Malkus and co-workers when the the resulting mass matrix was positive semi-definite (with zero masses), but generalization of these techniques to the indefinite case (with negative masses) was in progress at the time the current grant expired.

Publications

Journal and Reviewed Proceeding Articles Appearing or Accepted During Reporting Period

- D. S. Malkus, J. A. Nohel, and B. J. Plohr, Time-dependent shear flow of a non-Newtonian fluid, *Current Progress in Hyperbolic Systems: Riemann Problems and Computations*, B. Lindquist (Ed), *Contemporary Mathematics*, Vol. 100, Amer. Math. Soc. (1989), 91--109.
- D. S. Malkus, J. A. Nohel, and B. J. Plohr, Dynamics of shear flow a non-Newtonian fluid, *Journal of Computational Physics* 87(2) (1990), 464--487.
- M. Yao and D. S. Malkus, Boundary Node Correction and Superconvergence in the FEM, *Int. J. Num. Meths. Fluids* 10 (1990), 713--721.
- M. Yao and D. S. Malkus, Cancellation of Errors in the Higashitani Pritchard Treatment of Hole Pressures Generated by Viscoelastic Liquids in Creeping Flow Past a Transverse Slot, *Rheological Acta* 29 (1990), 310—322.
- D. S. Malkus, J. A. Nohel, and B. J. Plohr, Analysis of spurt phenomena for a non-Newtonian fluid, in *Problems Involving Change of Type* (ed. K. Kirchgässner), *Lecture Notes in Physics*, Vol. 359 (1990), 112-132, Springer-Verlag.
- D. S. Malkus, J. A. Nohel, and B. J. Plohr, Quadratic dynamical systems describing shear flow of non-Newtonian fluids, in *Nonlinear Evolution Equations That Change Type* (eds. Barbara L. Keyfitz, Michael Shearer), *The IMA Volumes in Mathematics and Its Applications*, Vol. 27 (1990), 146-163, Springer-Verlag.
- D. S. Malkus, J. A. Nohel, and B. J. Plohr, Analysis of new phenomena in shear flow of non-Newtonian fluids, *SIAM J. Appl. Math.* 51 (1991), 899-929.
- R. W. Kolkka, D. S. Malkus, and T. R. Rose, Finite rise time modeling of nearly monodisperse polymer melts and solutions, *Rheological Acta* 30 (1991), 430—446.

- D. Malkus, Y.-C. Tsai, and R. Kolkka, New Transient Algorithms for Non-Newtonian Flow, *Finite Elements in Fluids*, Vol. 8, Hemisphere Publishing Co., New York, in press.
- R. E. Cornwell and D. S. Malkus, Improved numerical dissipation for time integration algorithms in conduction heat transfer, *Comp. Meth. Appl. Mech. Eng.*, in press.

Thesis by Sponsored Research Assistant

Thermodynamics of Viscoelastic-Viscoplastic Materials, R. E. Cornwell, Dept. Engineering Mechanics, University of Wisconsin, 1991.

Books

- R. D. Cook, D. S. Malkus, and M. E. Plesha, *Concepts and Applications of Finite Element Analysis*, Third Edition, Wiley, 1989.

Interactions

Spoken Papers Presented at Meetings, Conferences, Seminars, etc.

- Midwest Mechanics Conference, Houghton, Mich. August 13--16, 1989. Session Organizer (with M. E. Plesha).
- Dept Aerospace Engrg. & Mechs. Colloquium, University of Minnesota, Minneapolis, Jan. 19, 1990.
- Dept. Mathematics Colloquium, Illinois Institute of Technology, Nov., 1990.
- Society of Rheology Annual Meeting, Santa Fe, October, 1990. Session Organizer on **Processing Rheology and Numerical Methods** and presented a paper.

Consultative and Advisory Functions

- The P. I. is Chairman of the Executive Committee of the Rheology Research Center (U. W. - Madison). This provides a valuable opportunity to interact with a broad spectrum of researchers in non-Newtonian mechanics from Mathematics Chemistry, Engineering Mechanics, and Chemical Engineering.

- The P.I is an Affiliate Member of the Center for the Mathematical Sciences and a member of the CMS Committee planning a new Applied Mathematics Ph. D. program.
- The P.I is Co-coordinator of the Computational Mechanics Group, a group of graduate students from the College of Engineering (mostly, but not exclusively, from the Department of Engineering Mechanics) and four faculty advisors who share a common interest in computing solutions to problems of practical and theoretical interest arising in mechanics. Our research interests are broad and include
 - Structural dynamics with emphasis on aerospace structures;
 - Numerical simulation of thermographic stress analysis;
 - Geomechanics with emphasis on numerical modeling of the tribology of rock joints;
 - Numerical modeling of advanced materials, particularly composites;
 - Numerical solution of non-Newtonian flow problems;
 - Numerical solution of problems involving thin plates and shells;
 - Numerical modeling of fracture and plasticity.

Our research is interdisciplinary, and we have close connections with the Center for the Mathematical Sciences (CMS) and the Rheology Research Center. D. S. Malkus and M. E. Plesha are the group coordinators. The Computational Mechanics Group is a Working Group of CMS. The Center for Mathematical Sciences (formerly Mathematics Research Center), University of Wisconsin - Madison, is an interdisciplinary research center, sponsored by individuals and groups of investigators who obtain research grants from a variety of federal agencies, which include AFOSR, NSF, ARO, and ONR.